Kim A Sharp

List of Publications by Year
in descending order

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99	16,590	31976	33894
papers	citations	53 h-index	99 g-index

101	101	101	15792
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational Graphics Software for Interactive Docking and Visualization of Ligandâ€“Protein Complementarity. Journal of Chemical Information and Modeling, 2021, 61, 1427-1443.	5.4	2
2	DNA Conformational Changes Play a Force-Generating Role during Bacteriophage Genome Packaging. Biophysical Journal, 2019, 116, 2172-2180.	0.5	13
3	Water loading driven size, shape, and composition of cetyltrimethylammonium/hexanol/pentane reverse micelles. Journal of Colloid and Interface Science, 2019, 540, 207-217.	9.4	14
4	Companion Simulations and Modeling to NMR-Based Dynamical Studies of Proteins. Methods in Enzymology, 2019, 615, 1-41.	1.0	4
5	Measuring Entropy in Molecular Recognition by Proteins. Annual Review of Biophysics, 2018, 47, 41-61.	10.0	77
6	Entropy in molecular recognition by proteins. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 6563-6568.	7.1	139
7	On the ability of molecular dynamics force fields to recapitulate <scp>NMR</scp> derived protein side chain order parameters. Protein Science, 2016, 25, 1156-1160.	7.6	21
8	Unpacking the origins of in-cell crowding. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1684-1685.	7.1	19
9	Characterization of Cetyltrimethylammonium Bromide/Hexanol Reverse Micelles by Experimentally Benchmarked Molecular Dynamics Simulations. Langmuir, 2016, 32, 1674-1684.	3.5	23
10	Analysis of the size dependence of macromolecular crowding shows that smaller is better. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 7990-7995.	7.1	133
11	Translation of Ludwig Boltzmannâ€™s Paper â€œOn the Relationship between the Second Fundamental Theorem of the Mechanical Theory of Heat and Probability Calculations Regarding the Conditions for Thermal Equilibriumâ€•Sitzungberichte der Kaiserlichen Akademie der Wissenschaften. Mathematisch-Naturwissen Classe. Abt. II, LXXVI 1877, pp 373-435 (Wien. Ber. 1877, 76:373-435). Reprinted in Wiss. Abhandlungen, Vol. II, reprint 42, p. 164-223, Barth, Leipzig, 1909. Entropy, 2015, 17, 1971-2009.	2.2	74
12	Regulation of brain glutamate metabolism by nitric oxide and S-nitrosylation. Science Signaling, 2015, 8, ra68.	3.6	108
13	A Sharp Thermal Transition of Fast Aromatic-Ring Dynamics in Ubiquitin. Angewandte Chemie - International Edition, 2015, 54, 102-107.	13.8	31
14	On the relationship between NMR-derived amide order parameters and protein backbone entropy changes. Proteins: Structure, Function and Bioinformatics, 2015, 83, 922-930.	2.6	60
15	The remarkable hydration of the antifreeze protein Maxi: A computational study. Journal of Chemical Physics, 2014, 141, 22D510.	3.0	27
16	Protein Folding, Interrupted. Science, 2014, 343, 743-744.	12.6	4
17	Banding 2of NMR-derived methyl order parameters: Implications for protein dynamics. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2106-2117.	2.6	18
18	TCR Triggering by pMHC Ligands Tethered on Surfaces via Poly(Ethylene Glycol) Depends on Polymer Length. PLoS ONE, 2014, 9, e112292.	2.5	46

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19	Microscopic Insights into the NMR Relaxation-Based Protein Conformational Entropy Meter. Journal of the American Chemical Society, 2013, 135, 15092-15100.	13.7	123
20	Calculation of Molecular Entropies Using Temperature Integration. Journal of Chemical Theory and Computation, 2013, 9, 1164-1172.	5.3	9
21	Calculation of Configurational Entropy with a Boltzmannâ€“Quasiharmonic Model: The Origin of High-Affinity Proteinâ€“Ligand Binding. Journal of Physical Chemistry B, 2011, 115, 9461-9472.	2.6	55
22	Allostery in the lac operon: Population selection or induced dissociation?. Biophysical Chemistry, 2011, 159, 66-72.	2.8	9
23	Improved method of preparation of supported planar lipid bilayers as artificial membranes for antigen presentation. Microscopy Research and Technique, 2011, 74, 1174-1185.	2.2	6
24	A peek at ice binding by antifreeze proteins. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 7281-7282.	7.1	52
25	Water in the Half Shell: Structure of Water, Focusing on Angular Structure and Solvation. Accounts of Chemical Research, 2010, 43, 231-239.	15.6	73
26	The Common Feature of Leukemia-Associated IDH1 and IDH2 Mutations Is a Neomorphic Enzyme Activity Converting Î±-Ketoglutarate to 2-Hydroxyglutarate. Cancer Cell, 2010, 17, 225-234.	16.8	1,754
27	Shape and evolution of thermostable protein structure. Proteins: Structure, Function and Bioinformatics, 2010, 78, 420-433.	2.6	17
28	Intrinsic Linear Heterogeneity of Amyloid Î² Protein Fibrils Revealed by Higher Resolution Mass-per-length Determinations. Journal of Biological Chemistry, 2010, 285, 41843-41851.	3.4	29
29	Protein Pockets: Inventory, Shape, and Comparison. Journal of Chemical Information and Modeling, 2010, 50, 589-603.	5.4	67
30	Building alternate protein structures using the elastic network model. Proteins: Structure, Function and Bioinformatics, 2009, 74, 682-700.	2.6	20
31	Influence of surface groups of proteins on water studied by freezing/thawing hysteresis and infrared spectroscopy. Biophysical Chemistry, 2009, 141, 222-230.	2.8	11
32	One Is Not Enough. Journal of Molecular Biology, 2009, 392, 1133-1144.	4.2	25
33	Finding and Characterizing Tunnels in Macromolecules with Application to Ion Channels and Pores. Biophysical Journal, 2009, 96, 632-645.	0.5	43
34	Thermophilic protein structure adaptation examined with Burial Depth and Travel Depth. Biophysical Journal, 2009, 96, 584a.	0.5	1
35	Explicit ion, implicit water solvation for molecular dynamics of nucleic acids and highly charged molecules. Journal of Computational Chemistry, 2008, 29, 1113-1130.	3.3	38
36	The Role of Conformation in Ion Permeation in a K⁺ Channel. Journal of the American Chemical Society, 2008, 130, 3389-3398.	13.7	32

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37	Re-Evaluation of the Model-Free Analysis of Fast Internal Motion in Proteins Using NMR Relaxation. Journal of Physical Chemistry B, 2008, 112, 12095-12103.	2.6	23
38	Surface-Anchored Monomeric Agonist pMHCs Alone Trigger TCR with High Sensitivity. PLoS Biology, 2008, 6, e43.	5.6	100
39	MAPPING COMPLICATED SURFACES ONTO A SPHERE. International Journal of Computational Geometry and Applications, 2007, 17, 305-329.	0.5	12
40	Temperature Dependence of Fast Dynamics in Proteins. Biophysical Journal, 2007, 92, L43-L45.	0.5	38
41	Atomic Charge Parameters for the Finite Difference Poissonâ^'Boltzmann Method Using Electronegativity Neutralization. Journal of Chemical Theory and Computation, 2006, 2, 1152-1167.	5.3	15
42	Proteinâ^'Solvent Interactions. Chemical Reviews, 2006, 106, 1616-1623.	47.7	137
43	Hydrogen Bonding and the Cryoprotective Properties of Glycerol/Water Mixtures. Journal of Physical Chemistry B, 2006, 110, 13670-13677.	2.6	250
44	Travel Depth, a New Shape Descriptor for Macromolecules: Application to Ligand Binding. Journal of Molecular Biology, 2006, 362, 441-458.	4.2	78
45	Pump-probe molecular dynamics as a tool for studying protein motion and long range coupling. Proteins: Structure, Function and Bioinformatics, 2006, 65, 347-361.	2.6	96
46	Hydrophobic tendency of polar group hydration as a major force in type I antifreeze protein recognition. Proteins: Structure, Function and Bioinformatics, 2005, 59, 266-274.	2.6	62
47	HEAT CAPACITY IN PROTEINS. Annual Review of Physical Chemistry, 2005, 56, 521-548.	10.8	384
48	Carbohydrate Intramolecular Hydrogen Bonding Cooperativity and Its Effect on Water Structure. Journal of Physical Chemistry B, 2005, 109, 24152-24159.	2.6	128
49	Implementation and testing of stable, fast implicit solvation in molecular dynamics using the smooth-permittivity finite difference Poisson-Boltzmann method. Journal of Computational Chemistry, 2004, 25, 2049-2064.	3.3	71
50	The mechanism of the type III antifreeze protein action: a computational study. Biophysical Chemistry, 2004, 109, 137-148.	2.8	65
51	Vibrational Stark Effects on Carbonyl, Nitrile, and Nitrosyl Compounds Including Heme Ligands, CO, CN, and NO, Studied with Density Functional Theory. Journal of Physical Chemistry B, 2004, 108, 6450-6457.	2.6	53
52	Analysis of thermal hysteresis protein hydration using the random network model. Biophysical Chemistry, 2003, 105, 195-209.	2.8	50
53	Solvent dependent and independent motions of COâ€"horseradish peroxidase examined by infrared spectroscopy and molecular dynamics calculations. Biophysical Chemistry, 2003, 106, 1-14.	2.8	14
54	Accessibility of oxygen with respect to the heme pocket in horseradish peroxidase. Proteins: Structure, Function and Bioinformatics, 2003, 53, 656-666.	2.6	25

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55	A Density Functional Theory Study of Conformers in the Ferrous CO Complex of Horseradish Peroxidase with Distinct Feâ^'Câ^'O Configurations. Journal of Physical Chemistry B, 2003, 107, 1884-1892.	2.6	8
56	A New Angle on Heat Capacity Changes in Hydrophobic Solvation. Journal of the American Chemical Society, 2003, 125, 9853-9860.	13.7	152
57	On the calculation of absolute macromolecular binding free energies. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 10399-10404.	7.1	145
58	Optical Spectra of Fe(II) Cytochrome c Interpreted Using Molecular Dynamics Simulations and Quantum Mechanical Calculations. Journal of Physical Chemistry B, 2002, 106, 5561-5571.	2.6	27
59	Stability of macromolecular complexes. Proteins: Structure, Function and Bioinformatics, 2002, 48, 645-653.	2.6	85
60	Entropy–enthalpy compensation: Fact or artifact?. Protein Science, 2001, 10, 661-667.	7.6	384
61	Spectral Analysis of Cytochromec:Â Effect of Heme Conformation, Axial Ligand, Peripheral Substituents, and Local Electric Fields. Journal of Physical Chemistry B, 2001, 105, 282-286.	2.6	22
62	Hydration Heat Capacity of Nucleic Acid Constituents Determined from the Random Network Model. Biophysical Journal, 2001, 81, 1881-1887.	0.5	41
63	Water structure changes induced by hydrophobic and polar solutes revealed by simulations and infrared spectroscopy. Journal of Chemical Physics, 2001, 114, 1791-1796.	3.0	202
64	The Influence of Protein Environment on the Low Temperature Electronic Spectroscopy of Zn-Substituted Cytochromec. Journal of Physical Chemistry B, 2000, 104, 6932-6941.	2.6	39
65	Changes in water structure induced by a hydrophobic solute probed by simulation of the water hydrogen bond angle and radial distribution functions. Biophysical Chemistry, 1999, 78, 33-41.	2.8	46
66	Calculating the electrostatic properties of RNA provides new insights into molecular interactions and function. Nature Structural Biology, 1999, 6, 1055-1061.	9.7	196
67	The Effects of Protein Environment on the Low Temperature Electronic Spectroscopy of Cytochrome c and Microperoxidase-11. Journal of Physical Chemistry B, 1999, 103, 6334-6348.	2.6	44
68	Exploration of the Structural Features Defining the Conduction Properties of a Synthetic Ion Channel. Biophysical Journal, 1999, 76, 618-630.	0.5	72
69	Effect of charge interactions on the carboxylate vibrational stretching frequency in c-type cytochromes investigated by continuum electrostatic calculations and FTIR spectroscopy. Biophysical Chemistry, 1998, 71, 9-20.	2.8	11
70	The role of protonation and metal chelation preferences in defining the properties of mercury-binding coiled coils 1 1Edited by P. E. Wright. Journal of Molecular Biology, 1998, 280, 897-912.	4.2	121
71	Electrostatic Contributions to Heat Capacity Changes of DNA-Ligand Binding. Biophysical Journal, 1998, 75, 769-776.	0.5	120
72	Calculation of Electron Transfer Reorganization Energies Using the Finite Difference Poisson-Boltzmann Model. Biophysical Journal, 1998, 74, 1241-1250.	0.5	64

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73	Effect of the Protein Denaturants Urea and Guanidinium on Water Structure:â€‰A Structural and Thermodynamic Study. Journal of the American Chemical Society, 1998, 120, 10748-10753.	13.7	226
74	Protein Electric Field Effects on the CO Stretch Frequency of Carbonmonoxycytochromescas a Function of Carbonyl Tilting and Bending Investigated with a Continuum Electrostatic Approach. Journal of Physical Chemistry B, 1997, 101, 7364-7367.	2.6	13
75	Hydrophobic Effect, Water Structure, and Heat Capacity Changes. Journal of Physical Chemistry B, 1997, 101, 4343-4348.	2.6	141
76	Energetics of Cyclic Dipeptide Crystal Packing and Solvation. Biophysical Journal, 1997, 72, 913-927.	0.5	33
77	Molecular Origin of Hydration Heat Capacity Changes of Hydrophobic Solutes:Â Perturbation of Water Structure around Alkanes. Journal of Physical Chemistry B, 1997, 101, 11237-11242.	2.6	59
78	Empirical free energy calculations: a blind test and further improvements to the method 1 1Edited by F. E. Cohen. Journal of Molecular Biology, 1997, 268, 401-411.	4.2	76
79	Finite difference Poisson-Boltzmann electrostatic calculations: Increased accuracy achieved by harmonic dielectric smoothing and charge antialiasing. Journal of Computational Chemistry, 1997, 18, 268-276.	3.3	70
80	On the Decomposition of Free Energies. Journal of Molecular Biology, 1996, 263, 123-125.	4.2	35
81	Electrostatic interactions in hirudin-thrombin binding. Biophysical Chemistry, 1996, 61, 37-49.	2.8	48
82	A rapid method for calculating derivatives of solvent accessible surface areas of molecules. Journal of Computational Chemistry, 1995, 16, 1038-1044.	3.3	67
83	Decomposition of Interaction Free Energies in Proteins and Other Complex Systems. Journal of Molecular Biology, 1995, 254, 77-85.	4.2	85
84	Correlating solvation free energies and surface tensions of hydrocarbon solutes. Biophysical Chemistry, 1994, 51, 397-409.	2.8	109
85	How much is a stabilizing bond worth?. Trends in Biochemical Sciences, 1994, 19, 526-529.	7.5	18
86	Salt Effects on Ligand-DNA Binding. Journal of Molecular Biology, 1994, 238, 245-263.	4.2	184
87	Salt Effects on Protein-DNA Interactions. Journal of Molecular Biology, 1994, 238, 264-280.	4.2	160
88	On the calculation of pKas in proteins. Proteins: Structure, Function and Bioinformatics, 1993, 15, 252-265.	2.6	514
89	Electrostatic fields in antibodies and antibody/antigen complexes. Progress in Biophysics and Molecular Biology, 1992, 58, 203-224.	2.9	92
90	Analysis of the heat capacity dependence of protein folding. Journal of Molecular Biology, 1992, 227, 889-900.	4.2	108

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91	Electrostatic contributions to solvation energies: comparison of free energy perturbation and continuum calculations. Journal of the American Chemical Society, 1991, 113, 1454-1455.	13.7	197
92	Incorporating solvent and ion screening into molecular dynamics using the finite-difference Poisson-Boltzmann method. Journal of Computational Chemistry, 1991, 12, 454-468.	3.3	124
93	Protein folding and association: Insights from the interfacial and thermodynamic properties of hydrocarbons. Proteins: Structure, Function and Bioinformatics, 1991, 11, 281-296.	2.6	5,360
94	The electrostatic potential of B-DNA. Biopolymers, 1989, 28, 975-993.	2.4	267
95	Calculating the electrostatic potential of molecules in solution: Method and error assessment. Journal of Computational Chemistry, 1988, 9, 327-335.	3.3	1,017
96	Synthesis and application of a poly(ethylene glycol)-antibody affinity ligand for cell separations in aqueous polymer two-phase systems. Analytical Biochemistry, 1986, 154, 110-117.	2.4	88
97	Focusing of electric fields in the active site of Cu-Zn superoxide dismutase: Effects of ionic strength and amino-acid modification. Proteins: Structure, Function and Bioinformatics, 1986, 1, 47-59.	2.6	730
98	Calculation of the Electrophoretic Mobility of a Particle Bearing Bound Polyelectrolyte Using the Nonlinear Poisson-Boltzmann Equation. Biophysical Journal, 1985, 47, 563-566.	0.5	117
99	Electrostatic and electrokinetic potentials in two polymer aqueous phase systems. Journal of Colloid and Interface Science, 1984, 102, 1-13.	9.4	90